Density Estimation and Smoothing

Density Estimation

- Suppose we have a random sample $X_1, \ldots, X_n$ from a population with density f.
- Nonparametric density estimation is useful if we
  - want to explore the data without a specific parametric model
  - want to assess the fit of a parametric model
  - want a compromise between a parametric and a fully non-parametric approach
- A simple method for estimating f at a point x:

  $$\widehat{f}_n(x) = \frac{\text{no. of } X_i \text{ in } [x-h, x+h]}{2hn}$$

  for some small value of h
- This estimator has bias

  $$\text{Bias}(\widehat{f}_n(x)) = \frac{1}{2h} p_h(x) - f(x)$$

  and variance

  $$\text{Var}(\widehat{f}_n(x)) = \frac{p_h(x)(1-p_h(x))}{4h^2 n}$$

  with

  $$p_h(x) = \int_{x-h}^{x+h} f(u)du$$

- If f is continuous at x and $f(x) > 0$, then as $h \to 0$
  - the bias tends to zero;
  - the variance tends to infinity.
- Choosing a good value of h involves a *variance-bias tradeoff*.

Kernel Density Estimation

- The estimator $\widehat{f}_n(x)$ can be written as

  $$\widehat{f}_n(x) = \frac{1}{nh}\sum_{i=1}^{n} K\left(\frac{x-x_i}{h}\right)$$

  with

  $$K(u) = \begin{cases} 1/2 & \text{if } |u| < 1 \\ 0 & \text{otherwise} \end{cases}$$

- Other *kernel functions* K can be used; usually
  - K is a density function
  - K has mean zero
  - K has positive, finite variance σ_K^2

  Often K is symmetric.

- Common choices of K:

$K(u)$	Range	Name
$1/2$	$\|u\| < 1$	Uniform, Boxcar
$\frac{1}{\sqrt{2\pi}}e^{-u^2/2}$		Gaussian
$1-\|u\|$	$\|u\| < 1$	Triangular
$\frac{3}{4}(1-u^2)$	$\|u\| < 1$	Epanechnikov
$\frac{15}{16}(1-u^2)^2$	$\|u\| < 1$	Biweight

Mean Square Error for Kernel Density Estimators

- The bias and variance of a kernel density estimator are of the form

$$\begin{aligned}\text{Bias}(\widehat{f}_n(x)) &= \frac{h^2\sigma_K^2 f''(x)}{2} + O(h^4)\\ \text{Var}(\widehat{f}_n(x)) &= \frac{f(x)R(K)}{nh} + o\left(\frac{1}{nh}\right)\end{aligned}$$

  with

$$R(g) = \int g(x)^2 dx$$

  if $h \to 0$ and $nh \to \infty$ and f is reasonable.

- The pointwise asymptotic mean square error is

$$\text{AMSE}(\widehat{f}_n(x)) = \frac{f(x)R(K)}{nh} + \frac{h^4\sigma_K^4 f''(x)^2}{4}$$

  and the asymptotic mean integrated square error is

$$\text{AMISE}(\widehat{f}_n) = \frac{R(K)}{nh} + \frac{h^4\sigma_K^4 R(f'')}{4}$$

- The resulting asymptotically optimal bandwidths h are

$$\begin{aligned}h_0(x) &= \left(\frac{f(x)R(K)}{\sigma_K^4 f''(x)^2}\right)^{1/5} n^{-1/5}\\ h_0 &= \left(\frac{R(K)}{\sigma_K^4 R(f'')}\right)^{1/5} n^{-1/5}\end{aligned}$$

  with optimal AMSE and AMISE

$$\begin{aligned}\text{AMSE}_0(\widehat{f}_n(x)) &= \frac{5}{4}(\sigma_K f(x)R(K))^{4/5} f''(x)^{2/5} n^{-4/5}\\ \text{AMISE}_0(\widehat{f}_n) &= \frac{5}{4}(\sigma_K R(K))^{4/5} R(f'')^{1/5} n^{-4/5}\end{aligned}$$

Choosing a Bandwidth

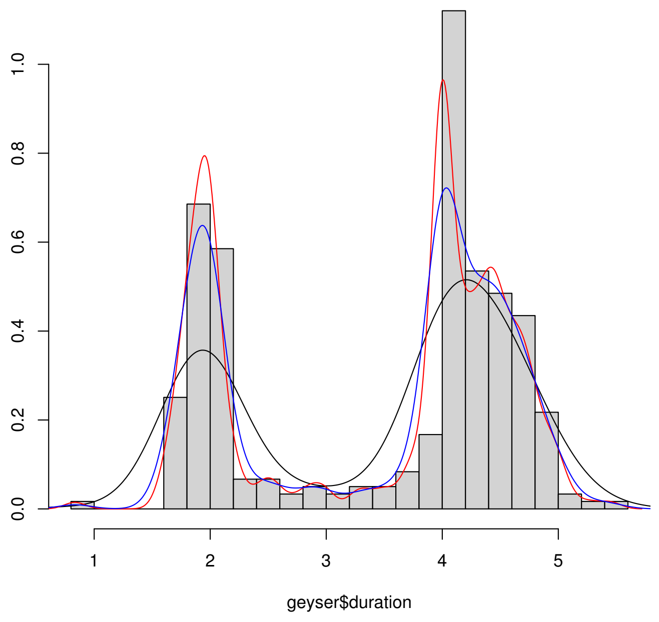
- One way to chose a bandwidth is to target a particular family, such as a Gaussian f:
  - The optimal bandwidth for minimizing AMISE when f is Gaussian and K is Gaussian
    $$h_0 = 1.059\sigma n^{-1/5}$$
  - σ can be estimated using S or the interquartile range
  - The default for `density` in R is
    $$0.9 \times \min(S, \text{IQR}/1.34) n^{-1/5}$$
    based on a suggestion of Silverman (1986, pp 45–47).
- This can often serve as a reasonable starting point.
- It does not adapt to information in the data that suggests departures from normality.
- So-called *plug-in* methods estimate $R(f'')$ to obtain
  $$\widehat{h} = \left(\frac{R(K)}{\sigma_K^4 \widehat{R(f'')}} \right)^{1/5} n^{-1/5}$$
- The Sheather-Jones method uses a different bandwidth (and kernel?) to estimate $\widehat{f}$ and then estimates $R(f'')$ by $R(\widehat{f}'')$.
- Specifying `bw="SJ"` in R's `density` uses the Sheather-Jones method. There are two variants:
  - `SJ-dpi`: direct plug-in
  - `SJ-ste`: solve the equation

  The default for `bw="SJ"` is `ste`.
- Other approaches based on leave-one-out cross-validation are available.
- Many of these are available as options in R's `density` and/or other density estimation functions available in R packages.
- Variable bandwidth approaches can be based on pilot estimates of the density produced with simpler fixed bandwidth rules.

Example: Durations of Eruptions of Old Faithful

- Based on an example in Venables and Ripley (2002).
- Durations, in minutes, of 299 consecutive eruptions of Old Faithful were recorded.
- The data are available as data set `geyser` in package `MASS`.
- Some density estimates are produced by

```
library(MASS)
data(geyser)
truehist(geyser$duration,nbin=25,col="lightgrey")
lines(density(geyser$duration))
lines(density(geyser$duration,bw="SJ"), col="red")
lines(density(geyser$duration,bw="SJ-dpi"), col="blue")
```



- Animation can be a useful way of understanding the effect of smoothing parameter choice. See files `tkdens.R`, `shinydens.R`, and `geyser.R` in

```
http://www.stat.uiowa.edu/~luke/classes/
          STAT7400/examples/
```

Also

```
http://www.stat.uiowa.edu/~luke/classes/
     STAT7400/examples/smoothex.Rmd
```

Issues and Notes

- Kernel methods do not work well at boundaries of bounded regions.
- Transforming to unbounded regions is often a good alternative.
- Variability can be assessed by asymptotic methods or by bootstrapping.
- A crude MCMC bootstrap animation:

```
g <- geyser$duration
for (i in 1:1000) {
    g[sample(299,1)] <- geyser$duration[sample(299,1)]
    plot(density(g,bw="SJ"),ylim=c(0,1.2),xlim=c(0,6))
    Sys.sleep(1/30)
}
```

- Computation is often done with equally spaced bins and fast Fourier transforms.
- Methods that adjust bandwidth locally can be used.
- Some of these methods are based on nearest-neighbor fits and local polynomial fits.
- Spline based methods can be used on the log scale; the `logspline` package implements one approach.

Density Estimation in Higher Dimensions

- Kernel density estimation can in principle be used in any number of dimensions.
- Usually a d-dimensional kernel K_d of the product form

$$K_d(u) = \prod_{i=1}^{d} K_1(u_i)$$

  is used.
- The kernel density estimate is then

$$\widehat{f}_n(x) = \frac{1}{n\det(H)} \sum_{i=1}^{n} K(H^{-1}(x-x_i))$$

  for some matrix H.
- Suppose $H = hA$ where $\det(A) = 1$. The asymptotic mean integrated square error is of the form

$$\text{AMISE} = \frac{R(K)}{nh^d} + \frac{h^4}{4}\int (\text{trace}(AA^T\nabla^2 f(x)))^2 dx$$

  and therefore the optimal bandwidth and AMISE are of the form

$$\begin{aligned} h_0 &= O(n^{-1/(d+4)}) \\ \text{AMISE}_0 &= O(n^{-4/(d+4)}) \end{aligned}$$

- Convergence is very slow if d is more than 2 or 3 since most of higher dimensional space will be empty—this is known as the *curse of dimensionality*.
- Density estimates in two dimensions can be visualized using perspective plots, surface plots, image plots, and contour plots.
- Higher dimensional estimates can often only be visualized by conditioning, or slicing.
- The `kde2d` function in package `MASS` provides two-dimensional kernel density estimates; an alternative is `bkde2D` in package `KernSmooth`.
- The `kde3d` function in the `misc3d` package provides three-dimensional kernel density estimates.

Example: Eruptions of Old Faithful

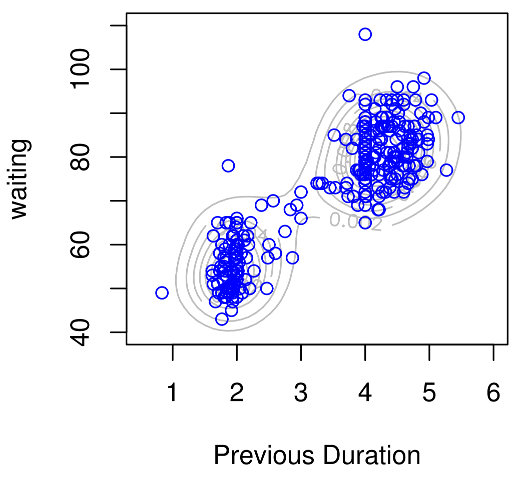
- In addition to duration times, waiting times, in minutes, until the following eruption were recorded.
- The duration of an eruption can be used to predict the waiting time until the next eruption.
- A modified data frame containing the previous duration is constructed by

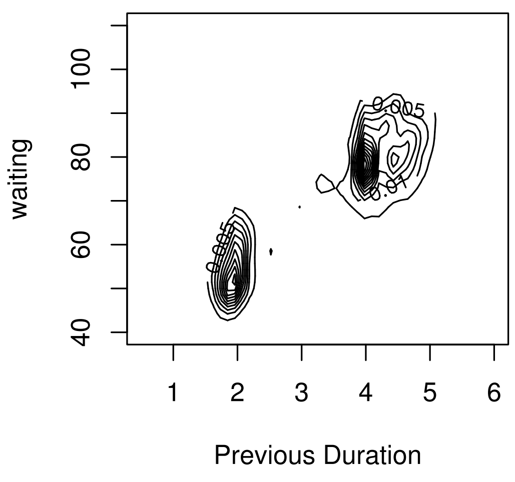
```
geyser2<-data.frame(as.data.frame(geyser[-1,]),
                    pduration=geyser$duration[-299])
```

- Estimates of the joint density of previous eruption duration and waiting time are computed by

```
kd1 <- with(geyser2,
            kde2d(pduration,waiting,n=50,lims=c(0.5,6,40,110)))
contour(kd1,col="grey",xlab="Previous Duration", ylab="waiting")
with(geyser2, points(pduration,waiting,col="blue"))
kd2 <- with(geyser2,
            kde2d(pduration,waiting,n=50,lims=c(0.5,6,40,110),
                  h=c(width.SJ(pduration),width.SJ(waiting))))
contour(kd2,xlab="Previous Duration", ylab="waiting")
```

Rounding of some durations to 2 and 4 minutes can be seen.



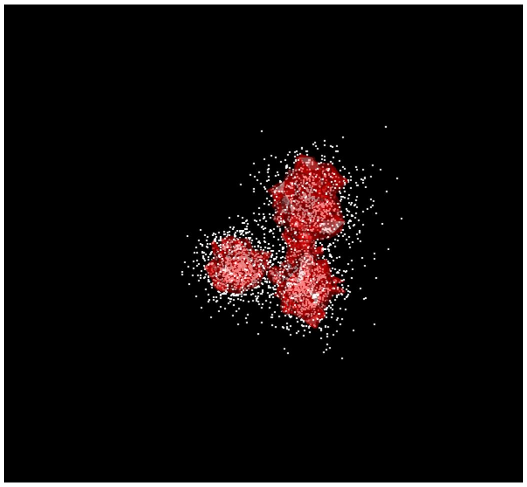


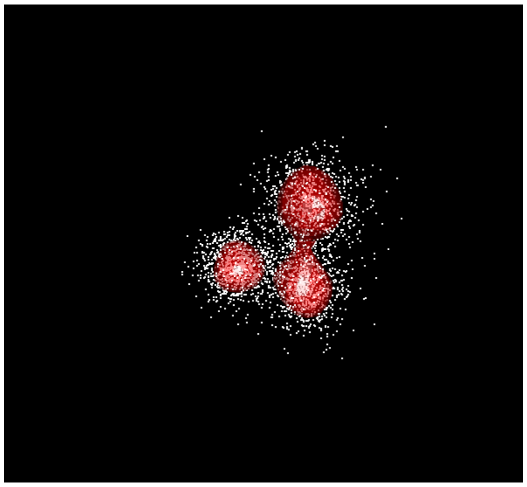
Visualizing Density Estimates

Some examples are given in `geyser.R` and `kd3.R` in

`http://www.stat.uiowa.edu/~luke/classes/STAT7400/examples/`

- Animation can be a useful way of understanding the effect of smoothing parameter choice.
- Bootstrap animation can help in visualizing uncertainty.
- For 2D estimates, options include
  - perspective plots
  - contour plots
  - image plots, with or without contours
- For 3D estimates contour plots are the main option
- Example: Data and contours for mixture of three trivariate normals and two bandwidths


BW = 0.2


BW = 0.5

Kernel Smoothing and Local Regression

- A simple non-parametric regression model is

$$Y_i = m(x_i) + \varepsilon_i$$

  with m a smooth mean function.

- A kernel density estimator of the conditional density $f(y|x)$ is

$$\widehat{f}_n(y|x) = \frac{\frac{1}{nh^2}\sum K\left(\frac{x-x_i}{h}\right)K\left(\frac{y-y_i}{h}\right)}{\frac{1}{nh}\sum K\left(\frac{x-x_i}{h}\right)} = \frac{1}{h}\frac{\sum K\left(\frac{x-x_i}{h}\right)K\left(\frac{y-y_i}{h}\right)}{\sum K\left(\frac{x-x_i}{h}\right)}$$

- Assuming K has mean zero, an estimate of the conditional mean is

$$\begin{aligned}\widehat{m}_n(x) = \int y\widehat{f}_n(y|x)dy &= \frac{\sum K\left(\frac{x-x_i}{h}\right)\int y\frac{1}{h}K\left(\frac{y-y_i}{h}\right)dy}{\sum K\left(\frac{x-x_i}{h}\right)}\\ &= \frac{\sum K\left(\frac{x-x_i}{h}\right)y_i}{\sum K\left(\frac{x-x_i}{h}\right)} = \sum w_i(x)y_i\end{aligned}$$

  This is the *Nadaraya-Watson* estimator.

- This estimator can also be viewed as the result of a *locally constant* fit: $\widehat{m}_n(x)$ is the value β_0 that minimizes

$$\sum w_i(x)(y_i - \beta_0)^2$$

- Higher degree local polynomial estimators estimate $m(x)$ by minimizing

$$\sum w_i(x)(y_i - \beta_0 - \beta_1(x-x_i) - \cdots - \beta_p(x-x_i)^p)^2$$

- Odd values of p have advantages, and $p = 1$, local linear fitting, generally works well.

- Local cubic fits, $p = 3$, are also used.

- Problems exist near the boundary; these tend to be worse for higher degree fits.

- Bandwidth can be chosen globally or locally.
- A common local choice uses a fraction of nearest neighbors in the x direction.
- Automatic choices can use estimates of σ and function roughness and plug in to asymptotic approximate mean square errors.
- Cross-validation can also be used; it often undersmooths.
- Autocorrelation creates an identifiability problem.
- Software available in R includes
  - `ksmooth` for compatibility with S (but much faster).
  - `locpoly` for fitting and `dpill` for bandwidth selection in package `KernSmooth`.
  - `lowess` and `loess` for nearest neighbor based methods; also try to robustify.
  - `supsmu`, Friedman's *super smoother*, a very fast smoother.
  - package `locfit` on CRAN

  All of these are also available for R; some are available as stand-alone code.

Spline Smoothing

- Given data $(x_1,y_1),\dots,(x_n,y_n)$ with $x_i \in [a,b]$ one way to fit a smooth mean function is to choose m to minimize

  $$S(m,\lambda) = \sum (y_i - m(x_i))^2 + \lambda \int_a^b m''(u)^2 du$$

  The term $\lambda \int_a^b m''(u)^2 du$ is a *roughness penalty*.

- Among all twice continuously differentiable functions on $[a,b]$ this is minimized by a *natural cubic spline* with *knots* at the x_i. This minimizer is called a *smoothing spline*.

- A *cubic spline* is a function g on an interval $[a,b]$ such that for some *knots* t_i with $a = t_0 < t_1 < \cdots < t_{n+1} = b$
  - on (t_{i-1}, t_i) the function g is a cubic polynomial
  - at $t_1,\dots,t_n$ the function values, first and second derivatives are continuous.

- A cubic spline is *natural* if the second and third derivatives are zero at a and b.

- A natural cubic spline is linear on $[a,t_1]$ and $[t_n,b]$.

- For a given λ the smoothing spline is a linear estimator.

- The set of equations to be solved is large but banded.

- The fitted values $\widehat{m}_n(x_i,\lambda)$ can be viewed as

  $$\widehat{m}_n(x,\lambda) = A(\lambda)y$$

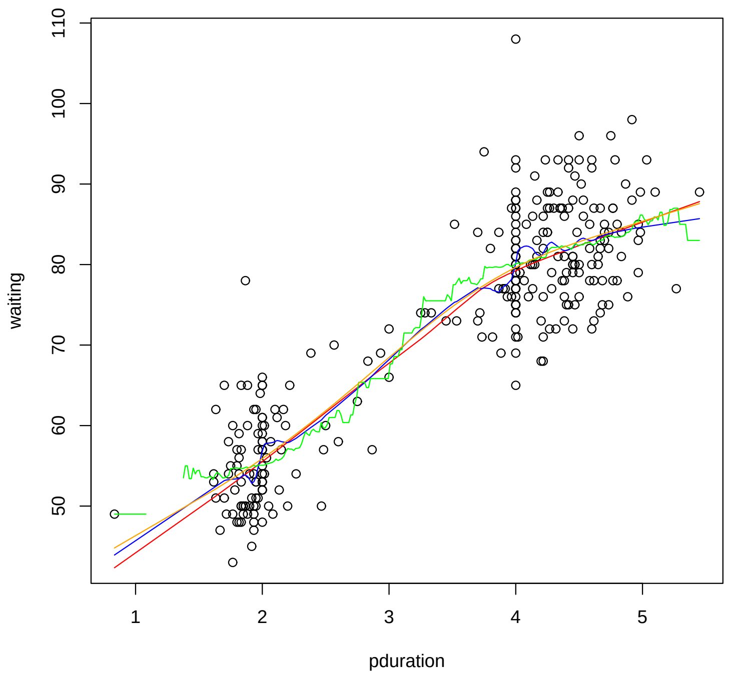
  where $A(\lambda)$ is the *smoothing matrix* or *hat matrix* for the linear fit.

- The function `smooth.spline` implements smoothing splines in R.

Example: Old Faithful Eruptions

- A nonparametric fit of waiting time to previous duration may be useful in predicting the time of the next eruption.
- The different smoothing methods considered produce the following:

```
with(geyser2, {
     plot(pduration,waiting)
     lines(lowess(pduration,waiting), col="red")
     lines(supsmu(pduration,waiting), col="blue")
     lines(ksmooth(pduration,waiting), col="green")
     lines(smooth.spline(pduration,waiting), col="orange")
})
```



- An animated version of the smoothing spline (available on line) shows the effect of varying the smoothing parameter.

Degrees of Freedom of a Linear Smoother

- For a linear regression fit with hat matrix

  $$H = X(X^T X)^{-1} X^T$$

  and full rank regressor matrix X

  $$\mathrm{tr}(H) = \text{number of fitted parameters} = \text{degrees of freedom of fit}$$

- By analogy define the degrees of freedom of a linear smoother as

  $$\mathrm{df}_{\mathrm{fit}} = \mathrm{tr}(A(\lambda))$$

  For the geyser data, the degrees of freedom of a smoothing spline fit with the default bandwidth selection rule are

```
> sum(with(geyser2,smooth.spline(pduration,waiting))$lev)
[1] 4.169843
> with(geyser2,smooth.spline(pduration,waiting))$df
[1] 4.169843
```

- For residual degrees of freedom the definition usually used is

  $$\mathrm{df}_{\mathrm{res}} = n - 2\mathrm{tr}(A(\lambda)) + \mathrm{tr}(A(\lambda)A(\lambda)^T)$$

- Assuming constant error variance, a possible estimate is

  $$\widehat{\sigma}_\varepsilon^2 = \frac{\sum(y_i - \widehat{m}_n(x_i,\lambda))^2}{\mathrm{df}_{\mathrm{res}}(\lambda)} = \frac{\mathrm{RSS}(\lambda)}{\mathrm{df}_{\mathrm{res}}(\lambda)}$$

- The simpler estimator

  $$\widehat{\sigma}_\varepsilon^2 = \frac{\mathrm{RSS}(\lambda)}{\mathrm{tr}(I - A(\lambda))} = \frac{\mathrm{RSS}(\lambda)}{n - \mathrm{df}_{\mathrm{fit}}}$$

  is also used.

- To reduce bias it may make sense to use a rougher smooth for variance estimation than for mean function estimation.

Choosing Smoothing Parameters for Linear Smoothers

- Many smoothing methods are linear for a given value of a smoothing parameter λ.
- Choice of the smoothing parameter λ can be based on leave-one-out cross-validation, i.e. minimizing the *cross-validation score*

$$\text{CV}(\lambda) = \frac{1}{n}\sum(y_i - \widehat{m}_n^{(-i)}(x_i,\lambda))^2$$

- If the smoother satisfies (at least approximately)

$$\widehat{m}_n^{(-i)}(x_i,\lambda) = \frac{\sum_{j\neq i} A(\lambda)_{ij} y_j}{\sum_{j\neq i} A(\lambda)_{ij}}$$

  and

$$\sum_{j=1}^{n} A(\lambda)_{ij} = 1 \quad \text{for all } i$$

  then the cross-validation score can be computed as

$$\text{CV}(\lambda) = \frac{1}{n}\sum\left(\frac{y_i - \widehat{m}_n(x_i,\lambda)}{1 - A_{ii}(\lambda)}\right)^2$$

- The *generalized cross-validation criterion*, or GCV, uses average leverage values:

$$\text{GCV}(\lambda) = \frac{1}{n}\sum\left(\frac{y_i - \widehat{m}_n(x_i,\lambda)}{1 - n^{-1}\text{trace}(A(\lambda))}\right)^2$$

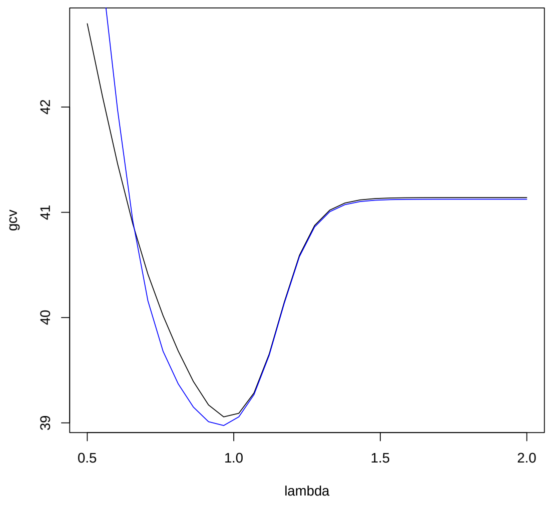
- The original motivation for GCV was computational; with better algorithms this is no longer an issue.

- An alternative motivation for GCV:
  - For an orthogonal transformation Q one can consider fitting $y_Q = QY$ with $A_Q(\lambda) = QA(\lambda)Q^T$.
  - Coefficient estimates and SS_{res} are the same for all Q, but the CV score is not.
  - One can choose an orthogonal transformation such that the diagonal elements of $A_Q(\lambda)$ are constant.
  - For any such Q we have $A_Q(\lambda)_{ii} = n^{-1}\text{trace}(A_Q(\lambda)) = n^{-1}\text{trace}(A(\lambda))$
- Despite the name, GCV does not generalize CV.
- Both CV and GCV have a tendency to undersmooth.

- For the geyser data the code

```
with(geyser2, {
    lambda <- seq(0.5,2,len=30)
    f <- function(s, cv = FALSE)
        smooth.spline(pduration,waiting, spar=s, cv=cv)$cv
    gcv <- sapply(lambda, f)
    cv <- sapply(lambda, f, TRUE)
    plot(lambda, gcv, type="l")
    lines(lambda, cv, col="blue")
})
```

extracts and plots GCV and CV values:



- Both criteria select a value of λ close to 1.

- Other smoothing parameter selection criteria include
  - Mallows C_p,
$$C_p = \text{RSS}(\lambda) + 2\widehat{\sigma}_\varepsilon^2 \text{df}_{\text{fit}}(\lambda)$$
  - Akaike's information criterion (AIC)
$$\text{AIC}(\lambda) = \log\{\text{RSS}(\lambda)\} + 2\text{df}_{\text{fit}}(\lambda)/n$$
  - Corrected AIC of Hurvich, Simonoff, and Tsai (1998)
$$\text{AIC}_C(\lambda) = \log\{\text{RSS}(\lambda)\} + \frac{2(\text{df}_{\text{fit}}(\lambda)+1)}{n - \text{df}_{\text{fit}}(\lambda) - 2}$$

Spline Representations

- Splines can be written in terms of many different bases,
  - B-splines
  - truncated power basis
  - radial or thin plate basis

  Some are more useful numerically, others have interpretational advantages.

- One useful basis for a cubic spline with knots $\{\kappa_1, \dots, \kappa_K\}$ is the *radial basis* or *thin plate basis*

$$1, x, |x-\kappa_1|^3, \dots, |x-\kappa_K|^3$$

- More generally, a basis for splines of order $2m-1$ is

$$1, x, \dots, x^{m-1}, |x-\kappa_1|^{2m-1}, \dots, |x-\kappa_K|^{2m-1}$$

  for $m = 1, 2, 3, \dots$.
  - $m = 2$ produces cubic splines
  - $m = 1$ produces linear splines

- In terms of this basis a spline is a function of the form

$$f(x) = \sum_{j=0}^{m-1} \beta_j x^j + \sum_{k=1}^{K} \delta_k |x-\kappa_k|^{2m-1}$$

- References:
  - P. J. Green and B. W. Silverman (1994). *Nonparametric Regression and Generalied Linear Models*
  - D. Ruppert, M. P. Wand, and R. J. Carroll (2003). *Semiparametric Regression*. `SemiPar` is an R package implementing the methods of this book.
  - G. Wahba (1990). *Spline Models for Observational Data.*
  - S. Wood (2017). *Generalized Additive Models: An Introduction with R, 2nd Ed.*. This is related to the `mgcv` package.

- A generic form for the fitted values is
$$\widehat{y} = X_0\beta + X_1\delta.$$
- *Regression splines* refers to models with a small number of knots K fit by ordinary least squares, i.e. by choosing β, δ to minimize
$$\|y - X_0\beta - X_1\delta\|^2$$
- *Penalized spline smoothing* fits models with a larger number of knots subject to a quadratic constraint
$$\delta^T D\delta \le C$$
for a positive definite D and some C.
- Equivalently, by a Lagrange multiplier argument, the solution minimizes the penalized least squares criterion
$$\|y - X_0\beta - X_1\delta\|^2 + \lambda\delta^T D\delta$$
for some $\lambda > 0$.
- A common form of D is
$$D = \left[|\kappa_i - \kappa_j|^{2m-1}\right]_{1\le i,j\le K}$$
- A variant uses
$$D = \Omega^{1/2}(\Omega^{1/2})^T$$
with
$$\Omega = \left[|\kappa_i - \kappa_j|^{2m-1}\right]_{1\le i,j\le K}$$
where the *principal square root* $M^{1/2}$ of a matrix M with SVD
$$M = U\text{diag}(d)V^T$$
is defined as
$$M^{1/2} = U\text{diag}(\sqrt{d})V^T$$
This form ensures that D is at least positive semi-definite.

- Smoothing splines are penalized splines of degree $2m-1=3$ with knots $\kappa_i = x_i$ and
$$D = \left[|\kappa_i - \kappa_j|^3\right]_{1 \le i,j \le n}$$
and the added natural boundary constraint
$$X_0^T \delta = 0$$
- For a natural cubic spline
$$\int g''(t)^2 dt = \delta^T D \delta$$
The quadratic form $\delta^T D \delta$ is strictly positive definite on the subspace defined by $X_0^T \delta = 0$.
- Penalized splines can often approximate smoothing splines well using far fewer knots.
- The detailed placement of knots and their number is usually not critical as long as there are enough.
- Simple default rules that often work well (Ruppert, Wand, and Carroll 2003):
  - knot locations:
$$\kappa_k = \left(\frac{k+1}{K+2}\right) \text{th sample quantile of unique } x_i$$
  - number of knots:
$$K = \min\left(\frac{1}{4} \times \text{ number of unique } x_i,\ 35\right)$$

  The `SemiPar` package actually seems to use the default
$$K = \max\left(\frac{1}{4} \times \text{ number of unique } x_i,\ 20\right)$$
- More sophisticated methods for choosing number and location of knots are possible but not emphasized in the penalized spline literature at this point.

A Useful Computational Device

To minimize
$$\|Y - X_0\beta - X_1\delta\|^2 + \lambda\delta^T D\delta$$
for a given λ, suppose B satisties
$$\lambda D = B^T B$$
and
$$Y^* = \begin{bmatrix} Y \\ 0 \end{bmatrix} \qquad X^* = \begin{bmatrix} X_0 & X_1 \\ 0 & B \end{bmatrix} \qquad \beta^* = \begin{bmatrix} \beta \\ \delta \end{bmatrix}$$
Then
$$\|Y^* - X^*\beta^*\|^2 = \|Y - X_0\beta - X_1\delta\|^2 + \lambda\delta^T D\delta$$
So $\widehat{\beta}$ and $\widehat{\delta}$ can be computed by finding the OLS coefficients for the regression of Y^* on X^*.

Penalized Splines and Mixed Models

- For strictly positive definite D and a given λ minimizing the objective function
$$\|y - X_0\beta - X_1\delta\|^2 + \lambda\delta^T D\delta$$
is equivalent to maximizing the log likelihood for the mixed model
$$Y = X_0\beta + X_1\delta + \varepsilon$$
with fixed effects parameters β and
$$\begin{aligned}\varepsilon &\sim \mathrm{N}(0, \sigma_\varepsilon^2 I)\\ \delta &\sim \mathrm{N}(0, \sigma_\delta^2 D^{-1})\\ \lambda &= \sigma_\varepsilon^2/\sigma_\delta^2\end{aligned}$$
with λ known.

- Some consequences:
  - The penalized spline fit at x is the BLUP for the mixed model with known mixed effects covariance structure.
  - Linear mixed model software can be used to fit penalized spline models (the R package `SemiPar` does this).
  - The smoothing parameter λ can be estimated using ML or REML estimates of σ_ε^2 and σ_δ^2 from the linear mixed model.
  - Interval estimation/testing formulations from mixed models can be used.

- Additional consequences:
  - The criterion has a Bayesian interpretation.
  - Extension to models containing smoothing and mixed effects are immediate.
  - Extension to generalized linear models can use GLMM methodology.

Example: Old Faithful Eruptions

- Using the function `spm` from `SemiPar` a penalized spline model can be fit with

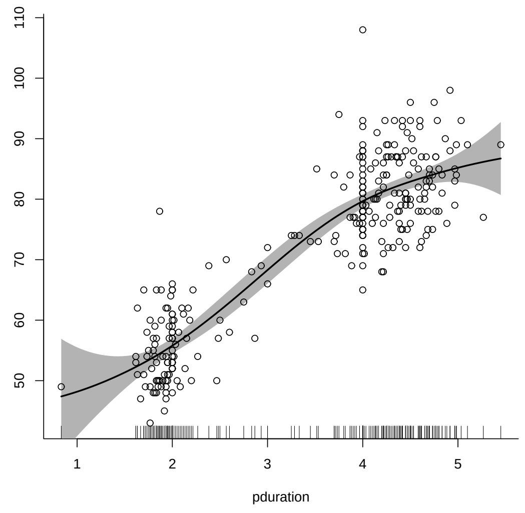
```
> library(SemiPar)
> attach(geyser2) # needed because of flaws in spm implementation
> summary(spm(waiting ~ f(pduration)))
Summary for non-linear components:

                df spar knots
f(pduration) 4.573  2.9    28

Note this includes 1 df for the intercept.
```

- The plot method for the `spm` result produces a plot with pointwise error bars:

```
> plot(spm(waiting ~ f(pduration)), ylim = range(waiting))
> points(pduration, waiting)
```



A fit using `mgcv`:

```
> library(mgcv)
> gam.fit <- gam(waiting ~ s(pduration), data = geyser2)
> summary(gam.fit)

Family: gaussian
Link function: identity

Formula:
waiting ~ s(pduration)

Parametric coefficients:
            Estimate Std. Error t value Pr(>|t|)
(Intercept)  72.2886     0.3594   201.1   <2e-16 ***
---
Signif. codes:  0 *** 0.001 ** 0.01 * 0.05 . 0.1   1

Approximate significance of smooth terms:
               edf Ref.df     F p-value
s(pduration) 3.149  3.987 299.8  <2e-16 ***
---
Signif. codes:  0 *** 0.001 ** 0.01 * 0.05 . 0.1   1

R-sq.(adj) =  0.801   Deviance explained = 80.3%
GCV = 39.046  Scale est. = 38.503    n = 298
```

A plot of the smooth component with the mean-adjusted waiting times is produced by

```
> plot(gam.fit)
> with(geyser2, points(pduration, waiting - mean(waiting)))
```

Smoothing with Multiple Predictors

- Many methods have natural generalizations
- All suffer from the curse of dimensionality.
- Generalizations to two or three variables can work reasonably.
- Local polynomial fits can be generalized to p predictors.
- `loess` is designed to handle multiple predictors, in principle at least.
- Spline methods can be generalized in two ways:
  - *tensor product splines* use all possible products of single variable spline bases.
  - *thin plate splines* generalize the radial basis representation.
- A thin plate spline of order m in d dimensions is of the form

  $$f(x) = \sum_{i=1}^{M} \beta_i \phi_i(x) + \sum_{k=1}^{K} \delta_k r(x - \kappa_k)$$

  with

  $$r(u) = \begin{cases} \|u\|^{2m-d} & \text{for } d \text{ odd} \\ \|u\|^{2m-d} \log \|u\| & \text{for } d \text{ even} \end{cases}$$

  and where the ϕ_i are a basis for the space of polynomials of total degree $\leq m-1$ in d variables. The dimension of this space is

  $$M = \binom{d+m-1}{d}$$

  If $d = 2, m = 2$ then $M = 3$ and a basis is

  $$\phi_1(x) = 1, \phi_2(x) = x_1, \phi_3(x) = x_2$$

Penalized Thin Plate Splines

- Penalized thin plate splines usually use a penalty with

  $$D = \Omega^{1/2}(\Omega^{1/2})^T$$

  where

  $$\Omega = \left[r(\kappa_i - \kappa_j)\right]_{1 \le i,j \le K}$$

  This corresponds at least approximately to using a squared derivative penalty.

- Simple knot selection rules are harder for $d > 1$.

- Some approaches:

  – space-filling designs (Nychka and Saltzman, 1998)

  – clustering algorithms, such as `clara`

Multivariate Smoothing Splines

- The bivariate smoothing spline objective of minimizing

  $$\sum(y_i - g(x_i))^2 + \lambda J(g)$$

  with

  $$J(g) = \int\int \left(\frac{\partial^2 g}{\partial x_1^2}\right)^2 + 2\left(\frac{\partial^2 g}{\partial x_1 \partial x_2}\right)^2 + \left(\frac{\partial^2 g}{\partial x_2^2}\right)^2 dx_1 dx_2$$

  is minimized by a thin plate spline with knots at the x_i and a constraint on the δ_k analogous to the natural spline constraint.
- Scaling of variables needs to be addressed
- Thin-plate spline smoothing is closely related to *kriging*.
- The general smoothing spline uses

  $$D = X_1 = [r(\kappa_i - \kappa_i)]$$

  with the constraint $X_0^T \delta = 0$.
- Challenge: the linear system to be solved for each λ value to fit a smoothing spline is large and not sparse.

Thin Plate Regression Splines

- Wood (2017) advocates an approach called *thin plate regression splines* that is implemented in the `mgcv` package.
- The approach uses the spectral decomposition of X_1
$$X_1 = UEU^T$$
with E the diagonal matrix of eigen values, and the columns of U the corresponding eigen vectors.
- The eigen values are ordered so that $|E_{ii}| \geq |E_{jj}|$ for $i \leq j$.
- The approach replaces X_1 with a lower rank approximation
$$X_{1,k} = U_k E_k U_k^T$$
using the k largest eigen values in magnitude.
- The implementation uses an iterative algorithm (Lanczos iteration) for computing the largest k eigenvalues/singular values and vectors.
- The k leading eigenvectors form the basis for the fit.
- The matrix X_1 does not need to be formed explicitly; it is enough to be able to compute $X_1 v$ for any v.
- k could be increased until the change in estimates is small or a specified limit is reached.
- As long as k is large enough results are not very sensitive to the particular value of k.
- `mgcv` by default uses $k = 10 \times 3^{d-1}$ for a d-dimensional smooth.

- This approach seems to be very effective in practice and avoids the need to specify a set of knots.
- The main drawback is that the choice of k and its impact on the basis used are less interpretable.
- With this approach the computational cost is reduced from $O(n^3)$ to $O(n^2k)$.
- For large n Wood (2017) recommends using a random sample of n_r rows to reduce the computation cost to $O(n_r^2 k)$. (From the help files the approach in `mgcv` looks more like $O(n \times n_r \times k)$ to me).

Example: Scallop Catches

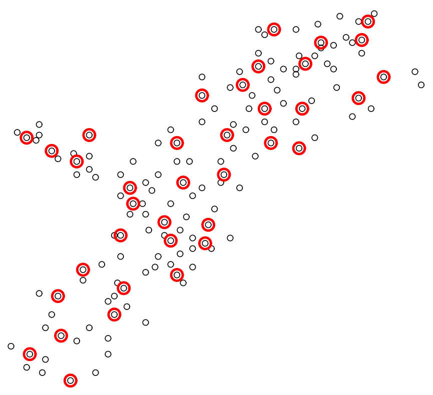
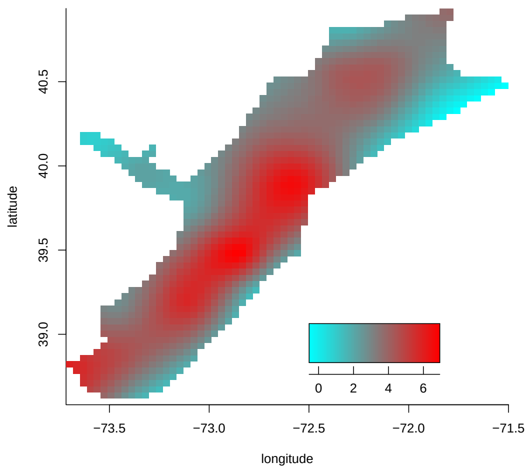
- Data records location and size of scallop catches off Long Island.
- A bivariate penalized spline fit is computed by

```
> data(scallop)
> attach(scallop)
> log.catch <- log(tot.catch + 1)
> fit <- spm(log.catch ~ f(longitude, latitude))
> summary(fit)

Summary for non-linear components:

                                df    spar knots
f(longitude,latitude) 25.12 0.2904    37
```

- Default knot locations are determined using `clara`
- Knot locations and fit:

A fit using `mgcv` would use

```
> scallop.gam <- gam(log.catch ~ s(longitude, latitude), data = scallop)
> summary(scallop.gam)

Family: gaussian
Link function: identity

Formula:
log.catch ~ s(longitude, latitude)

Parametric coefficients:
            Estimate Std. Error t value Pr(>|t|)
(Intercept)   3.4826     0.1096   31.77   <2e-16 ***
---
Signif. codes:  0 *** 0.001 ** 0.01 * 0.05 . 0.1   1

Approximate significance of smooth terms:
                        edf Ref.df     F p-value
s(longitude,latitude) 26.23  28.53 8.823  <2e-16 ***
---
Signif. codes:  0 *** 0.001 ** 0.01 * 0.05 . 0.1   1

R-sq.(adj) =  0.623   Deviance explained =   69%
GCV = 2.1793  Scale est. = 1.7784    n = 148
> plot(scallop.gam)
```

Computational Issues

- Algorithms that select the smoothing parameter typically need to compute smooths for many parameter values.
- Smoothing splines require solving an $n \times n$ system.
  - For a single variable the fitting system can be made tri-diagonal.
  - For thin plate splines of two or more variables the equations are not sparse.
- Penalized splines reduce the computational burden by choosing fewer knots, but then need to select knot locations.
- Thin plate regression splines (implemented in the `mgcv` package) use a rank k approximation for a user-specified k.
- As long as the number of knots or the number of terms k is large enough results are not very sensitive to the particular value of k.
- Examples are available in

```
http://www.stat.uiowa.edu/~luke/classes/
    STAT7400/examples/smoothex.Rmd
```